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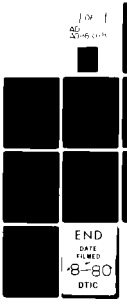

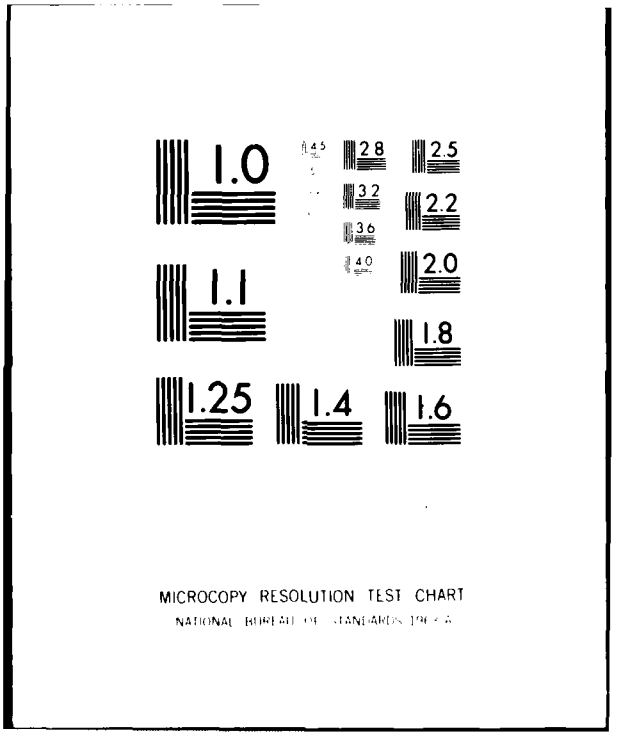
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ELECTRON CONDUCTIVITY IN COMBUSTION PLASMAS

L.C. PITCHFORD AND E.C. BEATY

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UNIVERSITY OF COLORADO
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The major uncertainty in the calculation of the conductivity in certain plasmas representative of those produced as combustion products in MHD generators is due to the uncertainty in the low energy momentum transfer cross sections for electron scattering in water vapor. The most reliable values of such low energy cross sections are those deduced from electron swarm experiments. The determination of cross sections from swarm experiments involves solving the Boltzmann equation for the electron energy distribution

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function using some assumed trial set of cross sections. Certain integrals of the distribution function yield the quantities measured in swarm experiments, such as drift velocities and diffusion coefficients. By comparing the calculated values of these measurable quantities with those found experimentally, it is possible to reach useful conclusions about the trial set of cross sections. An iterative procedure can then allow deduction of a set of cross sections which is consistent with swarm observations. The low energy cross sections are thus determined and are some of the most reliable available.

The conventional method of solving the Boltzmann equation in the context of electron swarm experiments relies on the approximation that the inelastic scattering cross sections are much smaller than the elastic. Because of the large dipole moment in H_2O, the rotational cross sections will be rather large and comparable to the elastic. Therefore, before attempting to determine cross sections in H_2O from swarm experiments, it has been necessary to improve on the solution and to evaluate the errors under some circumstances. This report details efforts in that direction and shows results for several cases using the extended analysis.

FOREWORD

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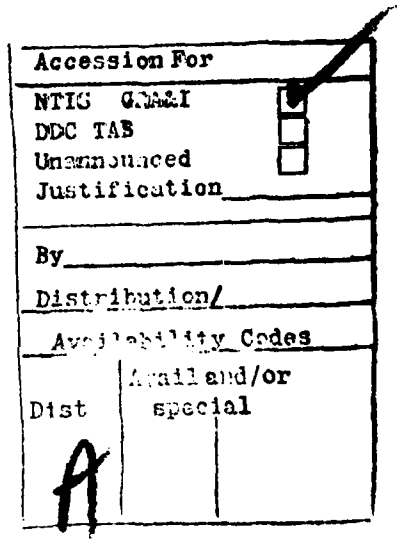

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SECTION I

INTRODUCTION

The major uncertainty in the calculation of the conductivity at a given temperature in certain plasmas representative of those produced as combustion products in MHD generators is due to the uncertainty in the low energy momentum transfer cross sections for electron scattering in water vapor.[1] The most reliable values of such low energy cross sections are those deduced from electron swarm experiments. The determination of cross sections from swarm experiments involves solving the Boltzmann equation for the electron energy distribution function using some trial set of assumed cross sections. Certain integrals of the distribution function yield the quantities measured in swarm experiments, such as drift velocities and diffusion coefficients. By comparing the calculated values of these measurable quantities with those found experimentally, it is possible to reach useful conclusions about the trial set of cross sections. An iterative procedure can then allow deduction of a set of cross sections which is consistent with swarm observations. The low energy cross sections are thus determined and are some of the most reliable.

The conventional method of solving the Boltzmann equation in the context of electron swarm experiments relies on the approximation that the inelastic scattering cross sections are much smaller than the elastic. Because of the large dipole moment in H_2O, the rotational cross sections will be rather large and comparable to the elastic. Therefore, before attempting to determine cross sections in H_2O from swarm experiments it has been necessary to improve on the solution and to evaluate the errors under some circumstances. This report details our efforts in that direction and shows results for several cases using the extended analyses.

The central problem is to deduce the distribution function from assumptions about the cross sections. The solution must be done numerically and in the course of the analysis it must be done many times. It is necessary to strike a balance between accuracy and required computer resources. The numerical problem is sufficiently difficult that it is necessary to involve assumptions which are of questionable validity such as the assumption of a nearly spherical electron energy distribution function. A major concern is the evaluation of the errors generated. Some of the errors arise because of physical assumptions which have the effect of changing the problem. In evaluating the error it is necessary to judge whether the simplified problem is similar enough to the initial problem. Another broad class of errors arises from inadequacies in the numerical analysis. The usual situation is that these errors depend on both the procedure and the data. For both classes of error we have made substantial progress in working out procedures with less error than before.

SECTION II

THE BOLTZMANN EQUATION

The motion of electrons traveling through a neutral gas under the influence of an electric field may be described mathematically by the Boltzman equation,

$$\frac{\partial f}{\partial t}(\vec{r},\vec{v},t) + \vec{v}\cdot\vec{\nabla}_r f(\vec{r},\vec{v},t) + \vec{a}\cdot\vec{\nabla}_v f(\vec{r},\vec{v},t) = c[f(\vec{r},\vec{v},t)] \qquad (1)$$

where $f(\vec{r},\vec{v},t)$ is the electron energy distribution function. The acceleration, $\vec{a}$, is that produced by the field ($\vec{a} = e\vec{E}/m$). The right hand side of the equation is the rate of change in the distribution function due to collisions. Since the only external force in the problem is a uniform electric field, the distribution function is cylindrically symmetric about the field direction.

Normally it is assumed the experimental situation is adequately described with the assumption that $f(\vec{r},\vec{v},t)$ is independent of position and time. These assumptions lead to the first two terms of Eq. (1) being zero. Actually, the configuration of the experiments imply spatial gradients which can also cause temporal variations. The impact of the density gradients on the distribution function is relatively small and can be found by a perturbative scheme proposed by Skullerud.[2] First, we discuss the spatially independent equation and its solutions.

With the assumption that the first two terms of Eq. (1) are negligible the Boltzmann equation becomes

$$\vec{a}\cdot\vec{\nabla}_v f^{(0)}(\vec{v}) - c[f^{(0)}(\vec{v})] = 0 \quad . \qquad (2)$$

where the collision term has the form,

$$c[f(\vec{v})] = -NvQ(v,\theta_s)f(\vec{v}) + \frac{N}{v^2}\sum_{k=o}\int v' f(\vec{v}')Q_k(v',\theta_s)\delta(v'-g(v))d^3v' \quad . \qquad (3)$$

The first term on the right of Eq. (3) represents scattering-out of the velocity volume d^3v element centered about v and the second term is the scattering-in component from all the volume elements d^3v' centered about v'. The symbols have the following meanings;

N = neutral particle density

$Q(v,\theta_s)$ = total scattering cross section

θ_s = scattering angle

$Q_k(v,\theta_s)$ = scattering cross section for the k^{th} process, k=0 for elastic scattering .

The delta functions serve the purpose of picking out those electrons of velocities v' that are scattered into d^3v after a collision of the k^{th} type. The integral over v' may be immediately performed given $g_k(v)$, the initial velocity v' in terms of the final velocity v. The $g_k(v)$'s will depend on the particular processes considered.

Since the energy loss in elastic collisions is small, the second term with k=0 may be expanded in a Taylor series about v and terms beyond $O(m/M)^2$ may be neglected. The resulting collision term is

$$
\begin{aligned}
&Nv\int [f(\omega',v) - f(\omega,v)]Q_o(v,\theta_s)d\omega' \\
&+ N\frac{1}{v^2}\frac{m}{M}\frac{\partial}{\partial v}\int (1-\cos\theta_s)Q_o(v,\theta_s)v^4 f(\omega',v)d\omega' \qquad (4)\\
&+ \sum_k Nv\int [f(\omega',v')\left(\frac{v'}{v}\right)^2 Q_k^{(*)}(v',\theta_s) - f(\omega,v)Q_k^{(*)}(v,\theta_s)]d\omega' \ .
\end{aligned}
$$

The sum is to be made over all inelastic and superelastic processes with cross sections Q_k and Q^*_k, respectively.

In order to convert the vector dependence of the single function f into the more easily handled scalar dependence of a coupled set of functions f_ℓ we expand f in terms of Legendre functions and the unknown coefficients f_ℓ

$$f(\vec{v}) = \sum_{\ell=o}^{n} f_\ell(v)P_\ell(\cos\theta) \ . \qquad (5)$$

For zero fields the distribution function must be spherically symmetric. At higher fields more terms are needed to represent the anisotropy in $f(\vec{v})$. Most work in the field has been done assuming that n=1 yields an adequate solution. This is referred to later as the two term solution. We do not constrain n to be small but in general find that n need not be larger than 7.

After substituting this expansion in Eq. (2), we multiply both sides by $P_j(\cos\theta)$ and integrate over all θ to yield $n+1 = N_p$ coupled differential equations for j=0, ... n. The coupling is between any three adjacent expansion coefficients according to the equation,

$$
\begin{aligned}
&- E\left\{\frac{j}{2j-1}\left[\varepsilon\frac{df_{j-1}(\varepsilon)}{d\varepsilon} - \frac{j-1}{2}f_{j-1}(\varepsilon)\right] + \frac{j+1}{2j+3}\left[\varepsilon\frac{df_{j+1}(\varepsilon)}{d\varepsilon} + \frac{j+2}{2}f_{j+1}(\varepsilon)\right]\right. \\
&= -N\varepsilon Q(\varepsilon)f_j(\varepsilon) + N\varepsilon f_j(\varepsilon)\int P_j(\cos\theta)Q_o(\varepsilon,\theta_s)d\omega' \\
&\quad +N\sum_k (\varepsilon\pm\varepsilon_k)f_j(\varepsilon\pm\varepsilon_k)\int P_j(\cos\theta_s)Q_k^{(*)}(\varepsilon\pm\varepsilon_k,\theta_s)d\omega' \\
&\quad - \text{recoil} = 0 \qquad j=0, \ldots n
\end{aligned}
\tag{6}
$$

In writing this equation we have made a change of variables to $\varepsilon = 1/2\ mv^2$ and have made use of the properties of Legendre functions. These equations are quite general so far and both superelastic and inelastic as well as anisotropic scattering may be explicitly included. In going from Eq. (2) to Eq. (6) a partial differential equation in two variables has been converted to N_p ordinary differential equations in one variable. The principal merit to this step comes from the fact that an adequate solution can be found with N_p relatively small.

SECTION III

METHOD OF SOLUTION

The set of first order differential equations (6) can be compactly expressed in matrix form as

$$A1(\varepsilon)F'(\varepsilon) + A0(\varepsilon)F(\varepsilon) + \sum_k A_k(\varepsilon \pm \varepsilon_k)F(\varepsilon \pm \varepsilon_k) = 0 \qquad (7)$$

where the elements of the column vector $F(\varepsilon)$ are the functions $f_\ell(\varepsilon)$ and the A's are square matrices of order N_p. The A's are matrices whose rows contain the coefficients appearing in Eq. (6). A1 and A0 are tridiagonal and the A_k's are purely diagonal.

The "non-local" terms, terms written as functions of $\varepsilon \pm \varepsilon_k$, appearing in Eqs. (6) and (7) are due to inelastic and superelastic collisions. It is the presence of these terms which preclude the use of common stepping methods of solution for differential equations. An approach (backward prolongation) taken by Frost and Phelps,[3] was to begin by assuming a solution for high energies, usually taken to be the solution for purely elastic scattering, and then stepping down to lower energies. If superelastic collisions are important it is necessary to know the solution at low energies in order to calculate it at high energies. A global approach is required in order to include the effect of the "non-local" terms in a general way. The particular method we have adopted is a type of collocation called Galerkin's method.[4]

To implement Galerkin's method, we make the additional expansion

$$\bar{F}(\varepsilon) = \sum_{j=1}^{N} C_j S_j(\varepsilon) \qquad (8a)$$

$$\text{with } F(\varepsilon) = \bar{F}(\varepsilon) + \delta(\varepsilon) \ . \qquad (8b)$$

C_j is a vector of length N_p and each element is by definition independent of energy. The $S_j(\varepsilon)$'s appearing in the expansion may be members of any convenient set of functions which is complete or nearly complete in the energy range of interest. $\delta(\varepsilon)$ is a small error accounting for the fact that a finite number of S_j's do not form a complete set of functions. In our work we choose the S_j's to be cubic B-splines.[5] Cubic B-splines are third degree polynomials with continuous first and second derivatives. A basis of such functions is local in the sense that at every energy point only a fixed number (four in the case of cubic splines) of B-splines is non-zero. B-splines are evaluated quite easily from their definition as a divided difference of the truncated power function[5] on some arbitrary energy grid, $\varepsilon_1, \ldots \varepsilon_{N_s}$.

A consequence of this choice of basis functions is that the distribution function is zero above ε_{N_s}. It is known that the distribution is small at high energies, and we can always choose an energy such that above it the distribution function is so small we are not interested. An important point to examine is that the calculated distribution function is independent of the high energy cut off point.

By combining (8a) and (7),

$$\sum_{j=1}^{N_s} C_j[A1(\varepsilon)S_j'(\varepsilon) + A0(\varepsilon)S_j(\varepsilon) + \sum_k A_k(\varepsilon\pm\varepsilon_k)S_j(\varepsilon\pm\varepsilon_k)] = \Delta(\varepsilon) \qquad (9)$$

where

$$\Delta(\varepsilon) = -[A1(\varepsilon)\delta'(\varepsilon) + A0(\varepsilon)\delta(\varepsilon) + \sum_k A_k(\varepsilon\pm\varepsilon_k)\delta(\varepsilon\pm\varepsilon_k)] \quad .$$

If $\Delta(\varepsilon)$ were zero for all ε, then the C_j's could be determined and would yield a solution $\bar{F}(\varepsilon) = F(\varepsilon)$. It is possible to approximate the ideal case

of vanishing $\Delta(\varepsilon)$ by forcing $\Delta(\varepsilon)$ to be outside the space spanned by $\{S_j\}$, that is by making $\Delta(\varepsilon)$ orthogonal to each S_i. Therefore we require

$$\langle S_i(\varepsilon)|\Delta(\varepsilon)\rangle = 0 \text{ for all } i = 1,\ldots,N_s \quad . \tag{10}$$

Using relation 10 in Eq. (9), we obtain

$$\sum_{j=1}^{N_s} C_j[\langle S_i(\varepsilon)|A1(\varepsilon)|S_j'(\varepsilon)\rangle + \langle S_i(\varepsilon)|A0(\varepsilon)|S_j(\varepsilon)\rangle \tag{11}$$

$$+ \langle S_i(\varepsilon)|\sum_k A_k(\varepsilon\pm\varepsilon_k)|S_j(\varepsilon\pm\varepsilon_k)\rangle] = 0$$

or in matrix form,

$$\underset{\sim}{M}\,\underset{\sim}{C} = 0 \tag{12}$$

with M_{ij} equal to the bracketed term in Eq. (11). The matrix M is a square matrix of order $N_p \times N_s$ but is rather sparse because only three splines are non-zero at any energy ε.

Eq. (10) is a set of homogeneous algebraic equations. To make the solution definite a further statement is required involving normalization. It is satisfactory to initially set

$$f_o(\varepsilon=0) = 1 \quad . \tag{13}$$

After solving the matrix equation the distribution function is renormalized to the condition

$$\int \varepsilon^{1/2} f_o(\varepsilon)d\varepsilon = 1 \quad .$$

The advantages of this method of solution are many. Most importantly, the non-local terms appearing in Eq. (11) and which are due to anisotropic scattering for $i>0$ are easily incorporated into the method. The calculation

of the elements of the matrix M are easy to perform using three to nine point Gauss-Legendre quadrature techniques. Many of the calculations including the method for solving Eq. (12) lend themselves well to the vector processing options available on the CRAY-1 computer that is being used for these calculations. The time required is thereby reduced to seconds per run. This method also allows for an unevenly spaced energy grid. However, since the error increases with the ratio of the maximum to the minimum energy interval spanned by any one B-spline, some care must be taken to optimize the grid selection. We commonly use $\varepsilon^{1/2}$ spacing. This seems to work quite well, although we suspect that it is not the optimum choice.

The main drawback to this method of solution is in the amount of computer storage required for the elements of the matrix M. No effort has been made so far to take advantage of the sparcity of M and the storage could be reduced by factors of two to ten or more when this is done. Most of the computing time is taken in determining the A1, A0 and A_k matrix elements. A significant reduction in time could be achieved by using some analytic form for cross sections to avoid the large numbers of interpolations required in the case of numerical cross section input.

The truncation of the Legendre series must be made after an even number of terms if recoil energy losses are neglected. This is because the number degrees of freedom is equal to the differential order of the system only for an even number of equations if there is no f_0' term (recoil) in the i=0 equation. When recoil is included, the f_0' term is present but with a very small coefficient. To avoid any stability problems that may occur, we always keep an even number of terms in the expansion.

The number of splines necessary to represent the distribution function adequately depend on the assumed data. We typically use about one hundred, although with some careful placement of the grid points, this number may be reduced. The choice of an optimum grid in collocation methods of this sort is a current topic of research among mathematicians and there are some mathematical guidelines for chosing the grid.[6] We intend to implement some of these ideas in the computer code and expect to cut down the number of energy grid points needed and therefore the size of the matrix M.

SECTION IV

TRANSPORT COEFFICIENTS

The transport coefficients are the measurable quantities in swarm experiments. It is these parameters that we wish to calculate to compare with the experiments and hence determine the set of cross sections that give the best fit between experiment and theory.

Once the distribution function $f(\vec{v})$ has been calculated, the drift velocity, W, is simply the component in the field direction of

$$\langle \vec{v} \rangle = \int \vec{v}\, f(\vec{v}) d^3v$$

$$\text{or} \qquad \langle v_z \rangle = W = \int v \cos\theta\, f(\vec{v}) d^3v \quad .$$

Because of the orthogonality of the Legendre functions

$$W = \frac{1}{3} \int v\, f_1(v) d^3v \tag{14}$$

Computation of the diffusion coefficients requires including the spatial dependence in the distribution function. Since spatial gradients of the electron density are small under conditions of swarm experiments, the spatial dependence may be included, following Skullerud,[2] in a perturbative way by expanding $f(\vec{r},\vec{v},t)$ in powers of the gradient of the electron density,

$$f(\vec{r},\vec{v},t) = \sum_{k=0} f^{(k)}(\vec{v}) \cdot (-\vec{\nabla})^k\, n(\vec{r},t) \tag{15}$$

$$= f^{(0)}(\vec{v}) n(\vec{r},t) - \vec{f}^{(1)}(\vec{v}) \cdot \vec{\nabla} n(\vec{r},t) + \ldots$$

When this is substituted into the Boltzmann equation,

$$n(\vec{r},t)\left\{\vec{a}\cdot\vec{\nabla}_v f^{(0)}(\vec{v}) - C[f^{(0)}(\vec{v})]\right\} \tag{16}$$

$$+ f^{(0)}(\vec{v})\frac{\partial n(\vec{r},t)}{\partial t} + \left\{f^{(0)}(\vec{v})\vec{v} + \vec{a}\cdot\vec{\nabla}_v \vec{f}^{(1)}(\vec{v})\right.$$

$$\left. - C[\vec{f}^{(1)}(\vec{v})]\right\} \cdot \vec{\nabla} n(\vec{r},t)$$

$$+ \ldots \qquad = 0 \quad .$$

The time dependence of the electron density can be expressed in terms of the transport coefficients, $\vec{\omega}^{(k)}$,

$$\frac{\partial n(\vec{r},t)}{\partial t} = \sum_{k=0} \vec{\omega}^{(k)} \cdot (-\vec{\nabla})^k n(\vec{r},t) \tag{17}$$

where

$\omega^{(0)} = 0$ -- no attachment or ionization

$\vec{\omega}^{(1)} = \vec{W}$ -- drift velocity

$\underset{\sim}{\omega}^{(2)} = \underset{\sim}{D}$ -- diffusion tensor

The first order solution already discussed is obtained by assuming $f(\vec{r},\vec{v},t) = f(\vec{v})$. Then from Eq. (16),

$$\vec{a} \cdot \vec{\nabla}_v f^{(0)}(\vec{v}) - C[f^{(0)}(\vec{v})] = 0 \quad . \tag{2}$$

Once Eq. (2) has been solved for $f^{(0)}(\vec{v})$, the second order solution is obtained by keeping two terms in expansion (15). The equation to solve for $\vec{f}^{(1)}(\vec{v})$ is

$$\vec{a} \cdot \vec{\nabla}_v \vec{f}^{(1)}(\vec{v}) - C[\vec{f}^{(1)}(\vec{v})] = (\vec{v}-\vec{W})f^{(0)}(\vec{v}) \quad . \tag{18}$$

This is a vector equation and, because of the cylindrical symmetry, there are only two independent components, one for $f_z^{(1)}(\vec{v})$ and the other for $f_x^{(1)}(\vec{v}) = f_y^{(1)}(\vec{v})$. Eq. (18) can be solved by the method outlined above as the right hand side is known.

The diffusion tensor $\underset{\sim}{D}$ may be written as

$$\underset{\sim}{D} = \frac{1}{N} \int \vec{v}\vec{f}^{(1)}(\vec{v}) d^3v$$

The components of interest are

$$D_p N = \int v_z f_z^{(1)}(\vec{v}) d^3v \text{ -- diffusion parallel to the field} \qquad (19a)$$

$$D_T N = \int v_x f_x^{(1)}(\vec{v}) d^3v \text{ -- diffusion perpendicular to the field} \qquad (19b)$$

It is D_T/μ and D_p/μ that are the measured quantities in the experiments and the relation to $D_T N$ or $D_p N$ is

$$\frac{D}{\mu} = \frac{DN(E/N)}{W} \quad . \qquad (20)$$

In what follows, our convergence criterion is based on values of W and D_T/μ as a function of the number of Legendre functions in the distribution function expansion rather than the distribution function itself since they are the measurables. We have not yet spent much effort on investigating the convergence of D_p/μ. D_T/μ is more commonly measured and the convergence of D_p/μ is expected to be similar to D_T/μ.

From the equations it can be seen that W and D_T/μ are functions of E/N and the neutral gas composition only. (This is in fact verified experimentally up to rather large neutral densities where the Boltzmann equation begins to break down.) By varying E/N, the experimenter is varying the average

energy of the electron swarm. When unfolding data from swarm experiments to determine cross sections, experiments and calculations are compared over as wide a range of E/N as possible, from near thermal average energies to the region of appreciable energy loss to ionization.

SECTION V

MODEL RESULTS

Many of the properties of the solution, in particular the convergence properties, can be seen most easily in simple model cases. In this section, we discuss the solutions for two model situations, a model atom and a methane model, each with one inelastic cross section, before going to the case of a real gas, nitrogen (N_2).

1. Model Atom

The simpliest model system we have looked at is that representative of a model atom. The cross sections for this model are illustrated in Fig. 1. The elastic cross section is constant at 6×10^{-16} cm^2 and the inelastic cross section is of the form $k(\varepsilon-\varepsilon_k)$, a ramp with a threshold energy at ε_k. The scattering is purely isotropic and superelastic collisions are not included. The neutral mass was taken to be 4 a.m.u.'s. The distribution function, W and D_T/μ were calculated for this model over a range of E/N from 1 to 48 Td (10^{-17} V cm^2), thresholds at .2 and 2 eV, and slopes for the inelastic cross section of 2 and 10×10^{-16} cm^2/eV. These values of input parameters are characteristic of distribution functions with average energies from a small fraction to several times the threshold energy.

Since the calculated values of transport coefficients are the quantities compared with experiment to determine the cross sections, it is these quantities with which we are most concerned. In particular, we would like to evaluate the error introduced by truncating the Legendre expansion for the distribution function after two terms as is usually done. To this end we have calculated values of W and $D_T N$ using as many terms in the Legendre expansion as are required for convergence.

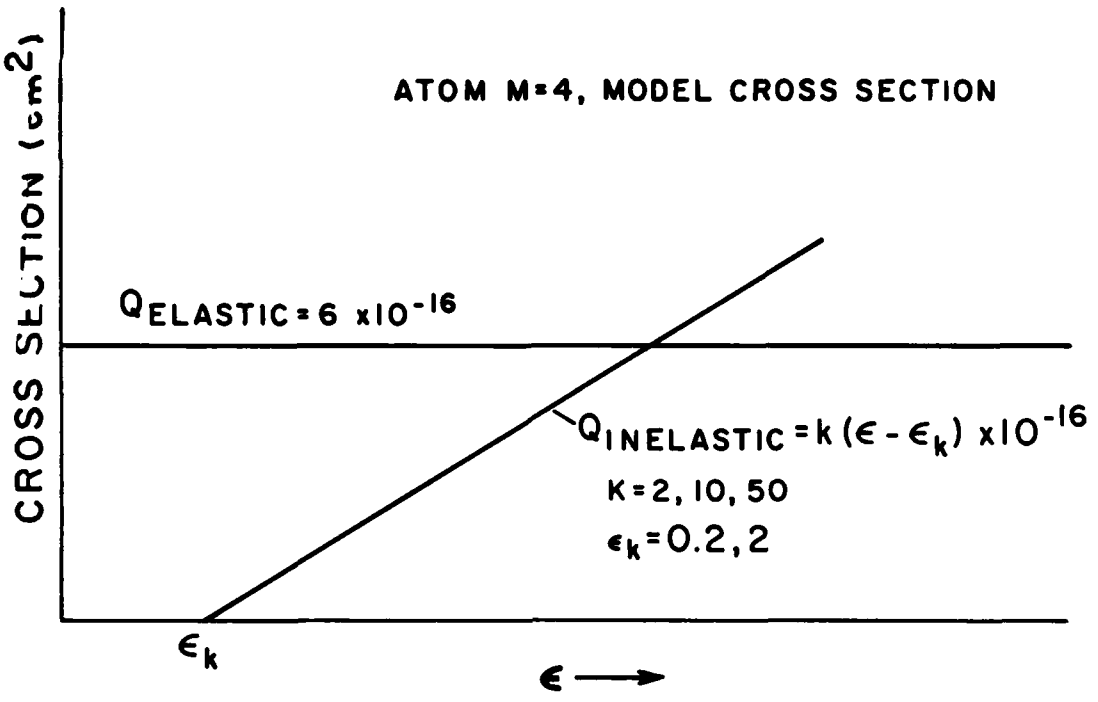

Figure 1. Model atom cross sections

The results of the calculations of W and D_T/μ as a function of E/N are shown for N_p=2 and N_p=6 in Fig. 2 for a value of $k = 10 \times 10^{-16}$ cm^2/eV. The two-term values are always greater than for N_p=6 and the difference between D_T/μ for Np=2 to N_p=4 was always much greater than the changes from N_p=4 to the largest value of N_p used. This indicates that the values of the transport coefficients have converged as a function of N_p.

We have compared values of W and D_T/μ with Monte Carlo calculations. The comparison with the six-term results is within the quoted accuracy[7] of the Monte Carlo results over the entire range of parameters investigated.

Although there are no physical significances to the Legendre expansion coefficients beyond the first, it is instructive to compare their magnitudes. Figure 3 is a plot of the f_i's for i=0 to 5 at an E/N of 24Td., ε_k = .2 eV, and $k = 10 \times 10^{-16}$ cm^2 eV. This is a case where the two term approximation clearly breaks down. The interesting features here are the zeros in the higher order coefficients occurring at successively higher energies and the maxima separated by approximately the same energy for $i \geq 2$. The most prominent feature is the similarity in the shapes of the f_i's on the high energy side of the zeros of the functions. The changes in f_0 and f_1 if going from two to six terms for the same model parameters are shown in Fig. 4. The dashed lines are the two term results. The two term results underestimate the final values at both the low and high energy ends while overestimating at the intermediate energies. This leads to the conclusion that the reaction rate coefficients calculated using the two term expansion tend to underestimate their true values.

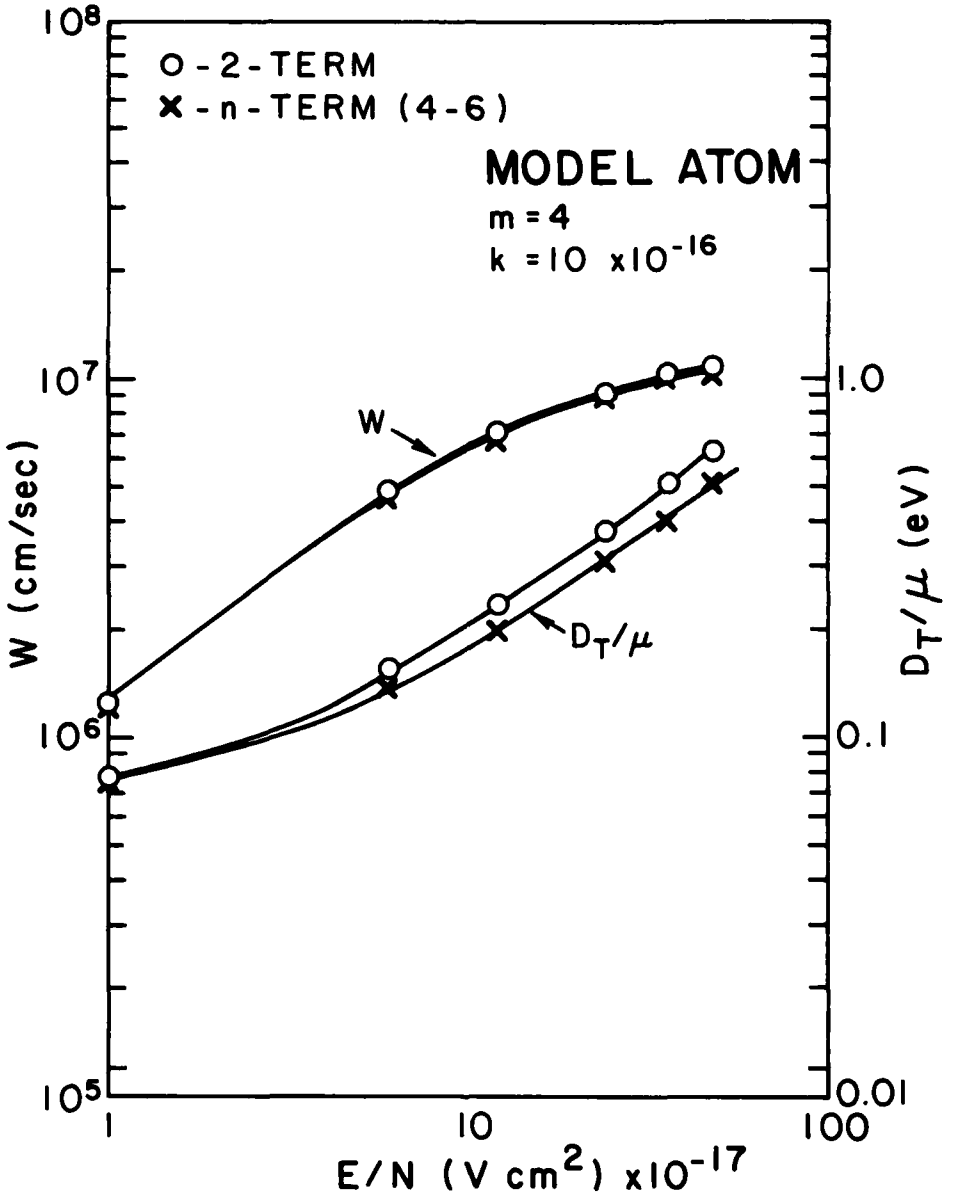

Figure 2. The transport coefficients W and D_T/μ as a function of E/N calculated for N_p=2 and N_p=6 in the model atom with k=10 x 10^{-16} cm^2 and ε_k=.2eV.

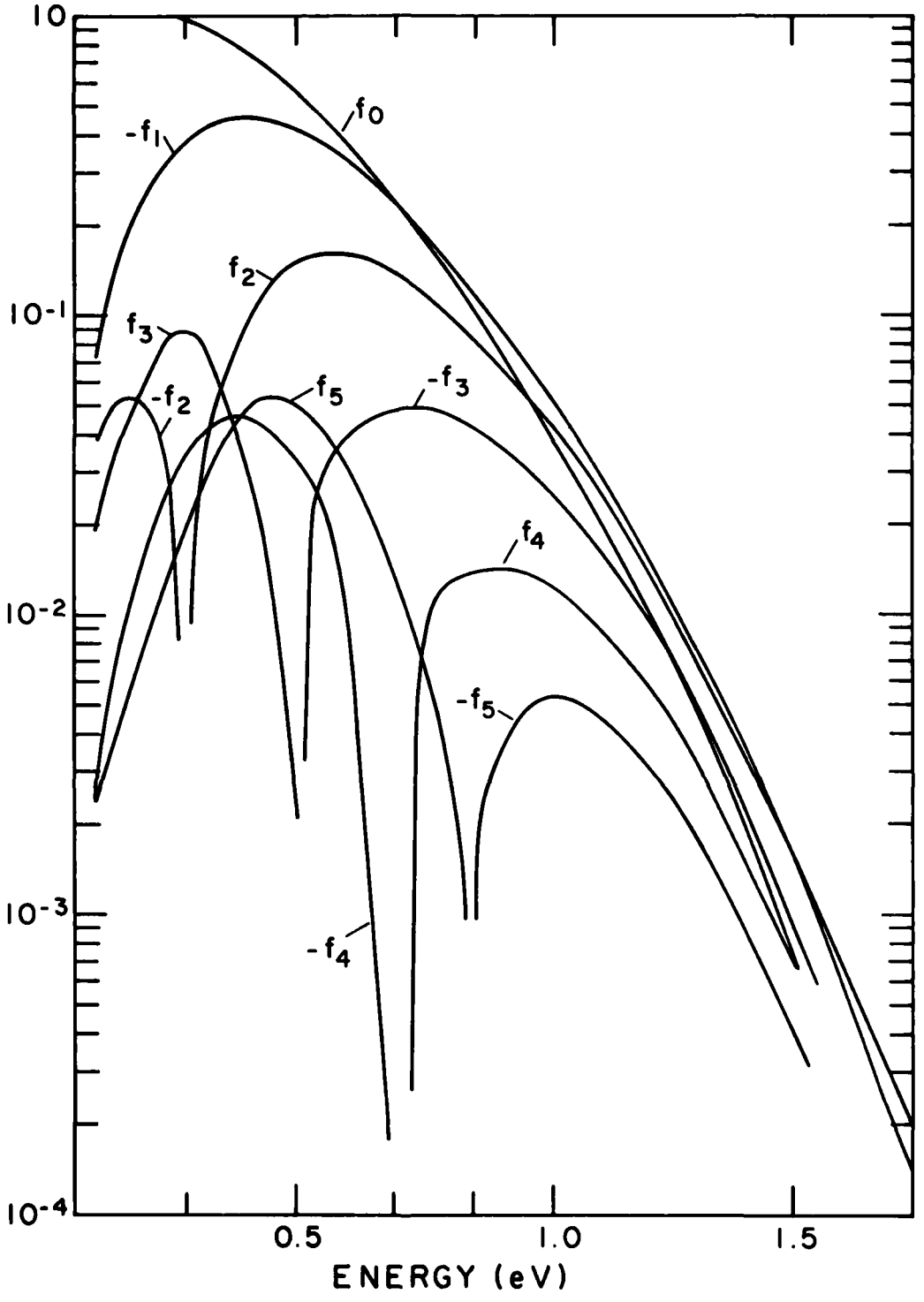

Figure 3. The first six Legendre expansion coefficients , f_i for i=0 to 5, as a function of energy for the model atom with E/N=24 Td, k=10 × 10^{-16} cm^2 / eV and ε_k=.2eV.

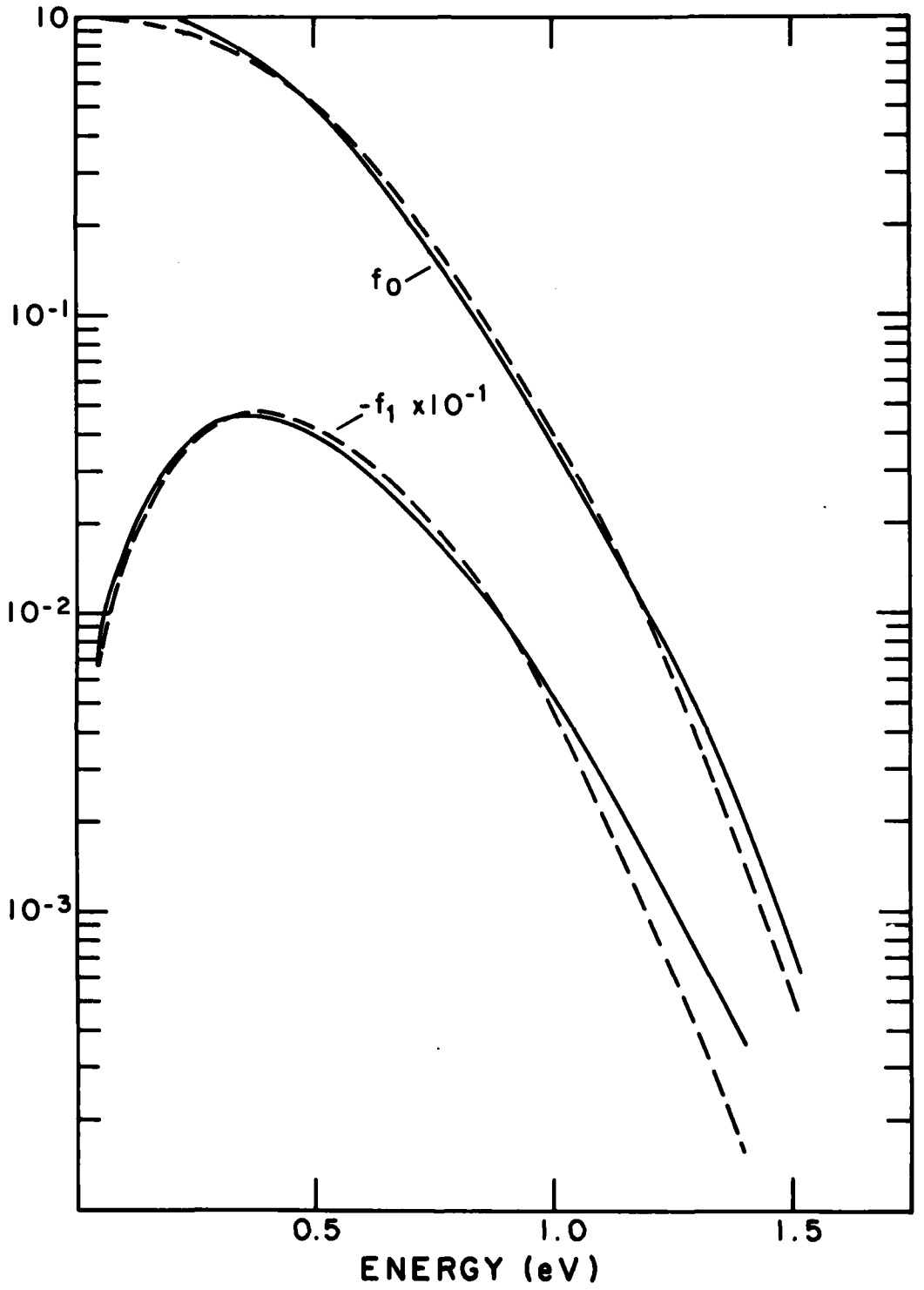

Figure 4. Comparison of f_o and f_1 from the two term and six term solutions. The solid lines are the N_p=6 solutions and the dashed lines are for N_p=2.

2. Methane

The cross sections adopted for these CH_4 calculations are as given by Kleban and Davis.[8] These cross sections shown as Fig. 5 are only meant to represent the gross features of the transport data and were not rigorously derived. We choose CH_4 for a detailed analysis because of the large value of the inelastic cross section in the region of the Ramsauer minimum in the elastic cross section. Based on the previously assumed criterion of a small ratio of inelastic to elastic cross sections, the two term analysis using these cross sections may be expected to exhibit severe departures from the multi-term analysis. This has indeed been the case.

The individual expansion coefficients f_i for i=0 to 5 are shown in Fig. 6 for E/N = 2.42 Td. The main features seen in the case of the model atom can also be seen here, i.e., the zeros and two maxima in the higher order coefficients. Figure 7 shows f_0 and f_1 for N_r=2 and N_r=6. As for the model atom, the two term solution tends to overestimate f_0 and f_1 for the intermediate energies and underestimates their values at higher energies.

Figure 8 shows results of calculations of W and D_T/μ for N=2 and N=6 over a range of E/N around the maximum in W. In no case is the two term value of D_T/μ within 5% of the multi-term results. Again as for the model atom, the change in going from Np=2 to 4 is larger than that from Np=4 to 6 or 8. We conclude that the two term analysis is inaccurate for CH_4 at this range of E/N and, although the error seems to be decreasing slightly as E/N is increased, there is probably no region where the two term solution in CH_4 is valid to better than 5%.

Monte Carlo calculations we have made in CH_4 verify our multi-term results for the transport coefficients. Lin, et al.[9] have developed a moment method for solving the Boltzmann equation which they applied to CH_4 using the present cross sections. We compare well with their published values at 3.9 Td.

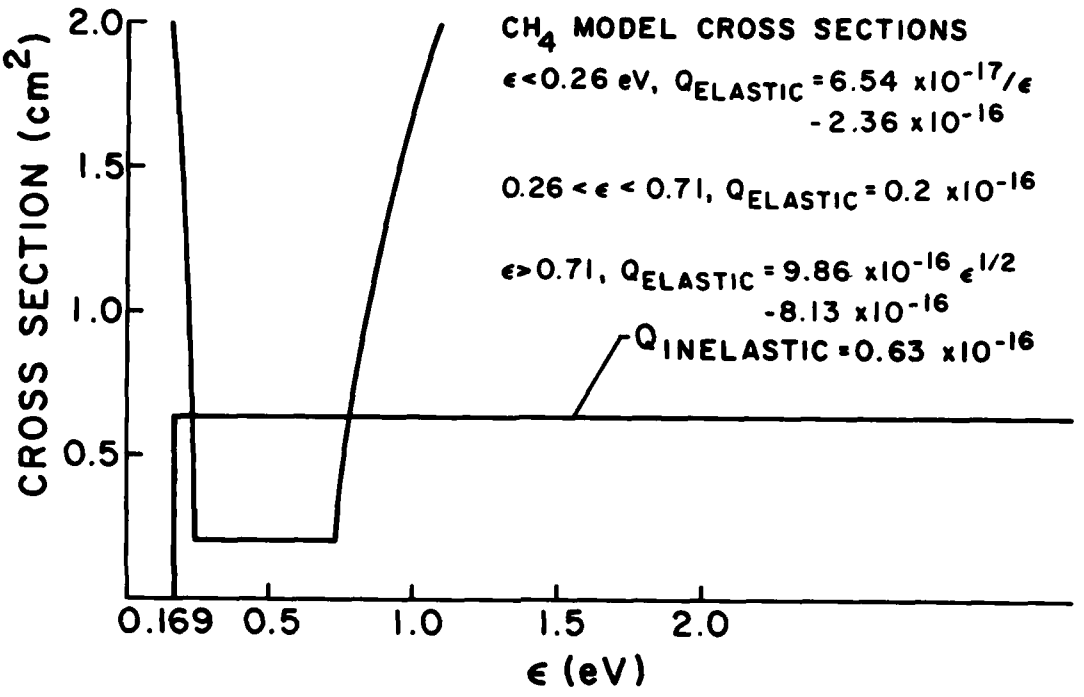

Figure 5. Methane cross sections used in the calculations.

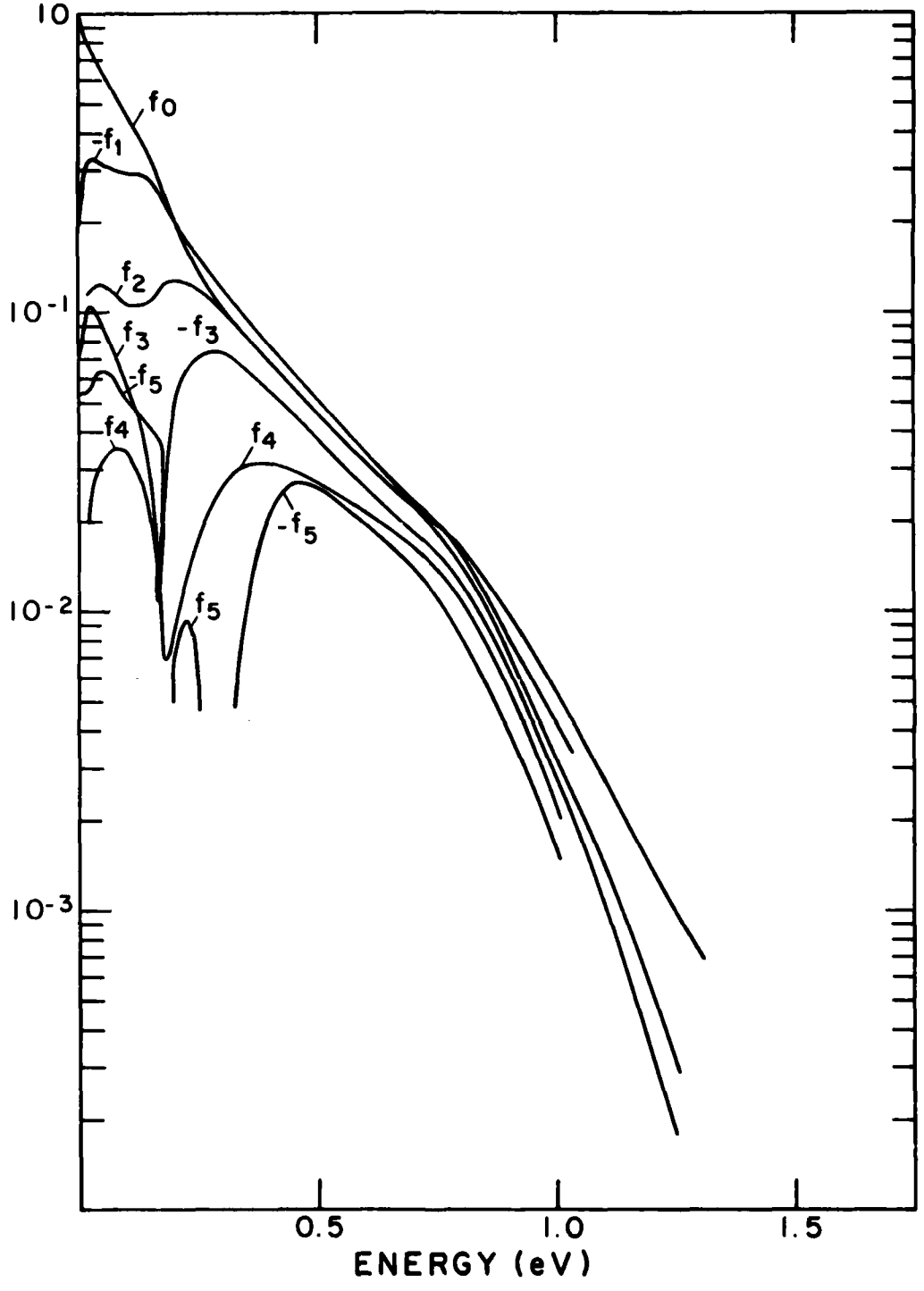

Figure 6. The first six Legendre expansion coefficients, f_i for i=0 to 5, as a function of energy for methane at 2.42 Td.

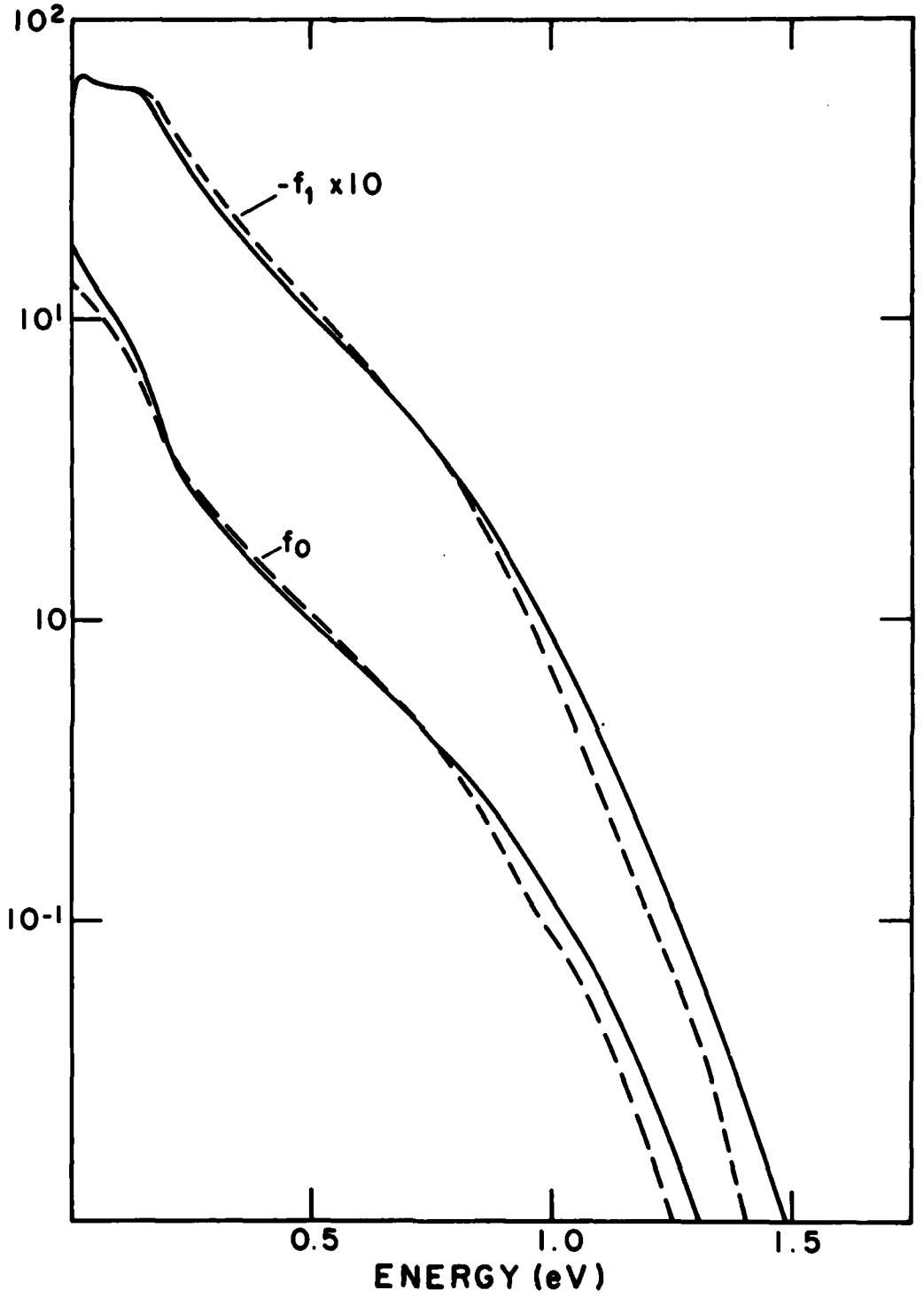

Figure 7. Comparison of f_o and f_1 from the two term and six term solutions. The solid lines are N_p =6 solutions and the dashed lines are for N_p=2.

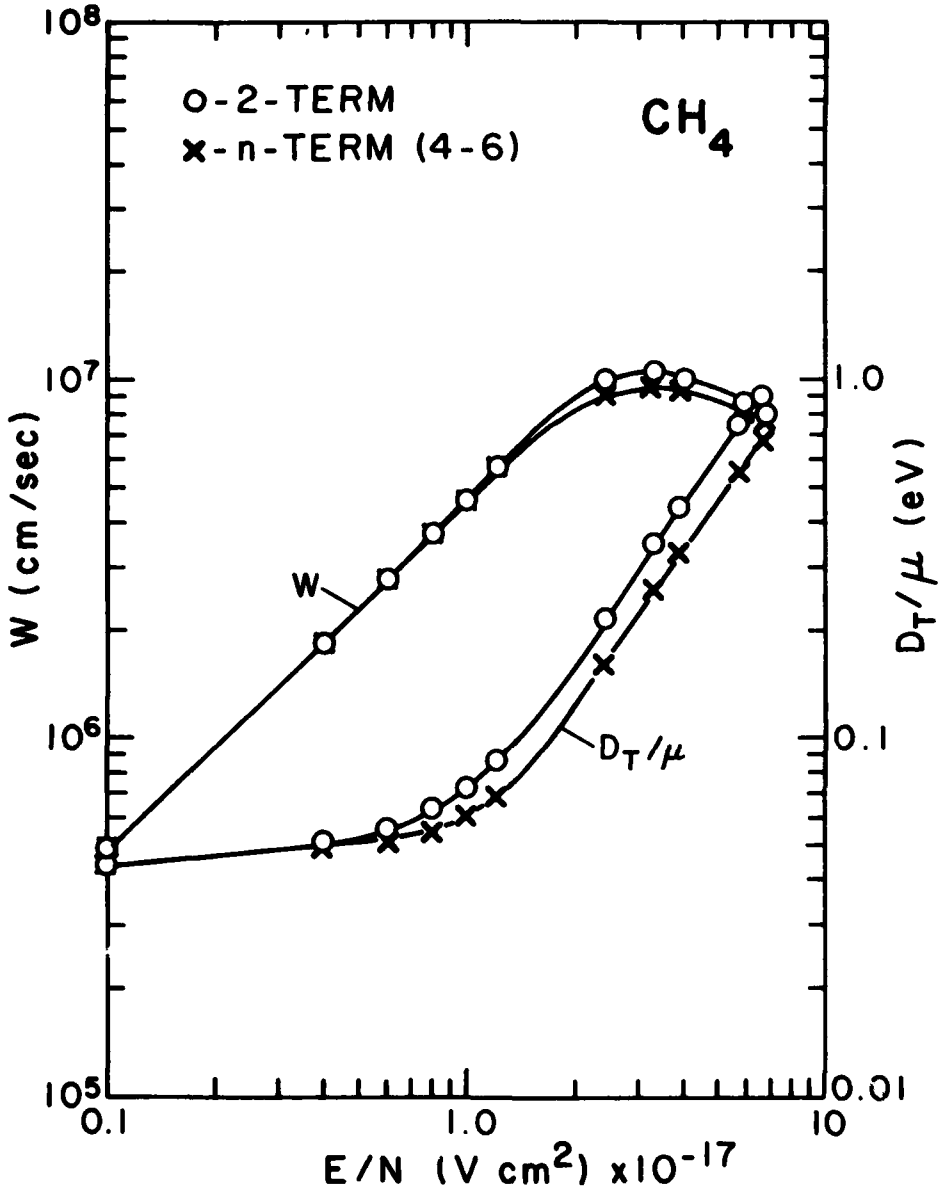

Figure 8. The transport coefficients W and D_T/μ as a function of E/N calculated for N_p=2 and N_p=6 in methane.

SECTION VI

NITROGEN RESULTS

The multi-term Boltzmann code has been used to calculate transport parameters in N_2 at 1, 40, and 100 Td. As input to the program, we use the set of cross sections in N_2 derived by Phelps.[10] Our point here is to evaluate the error introduced in the calculated W and $D_T N$ due to the two term expansion approximation and to compare with other methods.

We have made the calculations in N_2 using three different approximations in the Boltzmann code and using a Monte Carlo method. These different approximations were used with the Boltzmann approach to get some feeling for where each was more appropriate and easier to implement. These three approximations were all possible using our multi-term code. We have already discussed two of these in some detail, the two term and the multi-term approximations. A different approximation is due to Baraff.[11]

The Maximum Anisotropy Truncation (MAT) scheme proposed by Baraff [11] begins by assuming that the distribution function is highly elongated and an expansion in Legendre functions is very slowly converging if at all. If the angular dependence of $f(\vec{v})$ can be represented by a delta function, the relation between adjacent Legendre expansion coefficients is

$$f_i(\varepsilon) = \frac{2i+1}{2i-1} f_{i-1}(\varepsilon) \quad . \tag{21}$$

Rather than assuming that the higher order expansion coefficients can be neglected (f_i=0 for i>1) as in the traditional two-term Boltzmann analysis, the MAT truncation or uncoupling is based on Eq. (21). Baraff solves the two-term Boltzmann equation using Eq. 21 to substitute for f_2 in terms of f_1 in Eq. (6). We have implemented the MAT in our code and have solved the Boltzmann equation

keeping two terms and then six. If the higher order coefficients are indeed negligible, it should make no difference how the series is truncated but one method may require less terms than the other to converge. As will be seen, the series truncation by setting f_2=0 does yield two-term values closer to the converged results than the MAT scheme.

The Monte Carlo calculations were performed using the code provided by Ivan Reid and developed at the Australian National University.[7]

Table I shows the results of our calculations of W and D_TN using the four approaches discussed above. The first three rows of values for W and D_TN were computed by setting $f_{N_P} = 0$ in equation 6. A check of the N_p=2 results were made using the backward prolongation method.[3] As in the previously discussed model cases, the change in the values of W and D_TN in going from N_p=2 to N_p=4 are much greater than from N_p=4 to N_p=6. The differences between the N_p=2 and N_p=6 values are greater for higher values of E/N, as expected, and are greater for D_TN than for W.

The fourth and fifth rows are values calculated using the MAT assumption. There is a large difference between the two truncation methods for N_p=2 and a very small difference for the N_p=6 cases. This is to be expected if the series is converging. The MAT N_p=2 values are in substantial disagreement with the MAT N_p=6 values.

The last row contains values of W and D_TN calculated from a Monte Carlo method There are some discrepancies between the Boltzmann results and the Monte Carlo results at an E/N of 4.0×10^{-17} Vcm^2. We have reason to suspect that the Monte Carl code may be in error at the higher E/N values. For one thing, between collisions in the Monte Carlo code, the electrons travel in straight lines. The effect

TABLE 1

N_2 Drift Velocity - W

E/N	$= 1\times10^{-17}$ V cm^2	4×10^{-16} V cm^2	1×10^{-15} V cm^2
N_p=2	4.118×10^{5}cm sec^{-1}	5.640×10^{6}cm sec^{-1}	1.111×10^{7}cm sec^{-1}
N_p=4	4.118	5.560	1.096
N_p=6	4.118	5.558	1.096
MAT N_p=2	4.149	6.177	1.286
MAT N_p=6	4.118	5.559	1.105
Monte Carlo	4.12	5.42	1.083

N_2 Diffusion Coefficients - D_TN

E/N	$= 1\times10^{-17}$ V cm^2	4×10^{-16} V cm^2	1×10^{-15} V cm^2
N_p=2	1.323×10^{22}cm^{-1}sec^{-1}	1.744×10^{22}cm^{-1}sec^{-1}	2.035×10^{22}cm^{-1}sec^{-1}
N_p=4	1.317	1.624	1.822
N_p=6	1.319	1.630	1.850
MAT N_p=2	1.326	1.758	1.953
MAT N_p=6	1.317	1.612	1.852
Monte Carlo	1.305	1.604	1.901

of the field is to curve the electron trajectories. The straight line paths may tend to reduce the calculated drift velocities, and this is what is seen when comparing with the Boltzmann code.

At this point it is not too instructive to compare computing speeds among the various methods. First, very little effort has been made to optimize the speed requirements in the Boltzmann code. The Monte Carlo calculations are very time consuming, but an exact figure on the savings using the Boltzmann code is not available yet. Presently factors of 10 to 1000 in speed are saved by using the Boltzmann code. Another point making a comparison difficult is the fact that we are using the vector processing facilities of the CRAY-1 computer. It is hard to estimate what execution times would be without that option.

SECTION VII

CONCLUSIONS

The determination of low energy electron scattering cross sections from swarm experiments has relied almost exclusively on the two term Boltzmann analysis up to now for the calculation of W and D_T/μ. This has generally been assumed valid for cases where the inelastic cross sections are much smaller than the elastic. We have presented here a method for generalizing the Boltzmann analysis to include an arbitrary number of terms in the Legendre expansion of the distribution function. The method has been applied to two model cases and to nitrogen as an example of a real gas with a large number of inelastic processes.

We find that, in general, the error introduced in the transport parameters calculated using the two term approximation is greater at higher ratios of inelastic to elastic cross sections. In the case of methane, the error decreases with decreasing ratio of cross sections yet increasing E/N. The error in D_TN for any particular case is always much larger than for W.

Agreement between other methods of our multi-term results are good. Comparison between the backward prolongation two term calculation and our code with N_P=2 is exact for all cases investigated. Our converged values of transport coefficients compare well with Monte Carlo results within quoted accuracies except for the higher E/N cases in N_2. The reason for the discrepancies is not understood. Finally, since this project began another multi-term Boltzmann method based on moment techniques has appeared in the literature.[9] We compare our results in CH_4 at 3.9 Td with the values published for W and D_TN as a function of N_P and find excellent agreement.

We have been concerned here that part of the swarm experiment analysis in which the Boltzmann equation is solved for the electron energy distribution function and hence the transport coefficients. The iterative determination of cross sections by comparison of calculated and measured values of W and D/μ is yet another issue about which only general remarks may be made. Kumar, Skullerud, and Robson[12] note that in order to glean maximum information from the potentially extremely accurate swarm measurements, we should aim for accuracies of .1% and 1% for W and $D_T N$, respectively, in the calculations. We have shown here that such accuracies can not be achieved using the two-term approximation. It is possible to show[13] that in helium, a 2% variation in the momentum transfer cross section leads to about a 2% change in the calculated drift velocity over a certain range of E/N, but it should be noted that the correspondence between change in cross sections and change in drift velocity is certainly not in general true.

The validity of the two term approximation has been debated and questioned for some time. If accuracies of .1% and 1% or less in W and $D_T N$, respectively, are desired from the calculations, the two term approximation is of limited validity. In N_2 at 40 Td, the two term W and $D_T N$ values differ from the six term values by 1.4 percent and 6.9 percent, respectively. At 100 Td, the differences are 1.6 percent and 10 percent, respectively. However, for 1 Td, the two term values seem quite accurate. In CH_4 the two term $D_T N$ is greater than 5 percent different from the six term value for all values of E/N investigated.

Attempts to quantify the error introduced by the two term approximation have met with limited success. We plan to continue these efforts in this direction, as some criteria for when the two term approximation is valid would be very useful.

A variety of problems may now be addressed using the code. One interesting problem is the behavior of the high energy tail of the distribution function as a function of the number of Legendre functions in the solution. This will hopefully resolve some of the problems encountered in determining electronic excitation or ionization rate coefficients simultaneously with the transport coefficients. Finally, with the method presented here, we may now return to the original problem of the analysis of the swarm experiments in water vapor to obtain more accurate values of the low energy electron-water molecule scattering cross sections.

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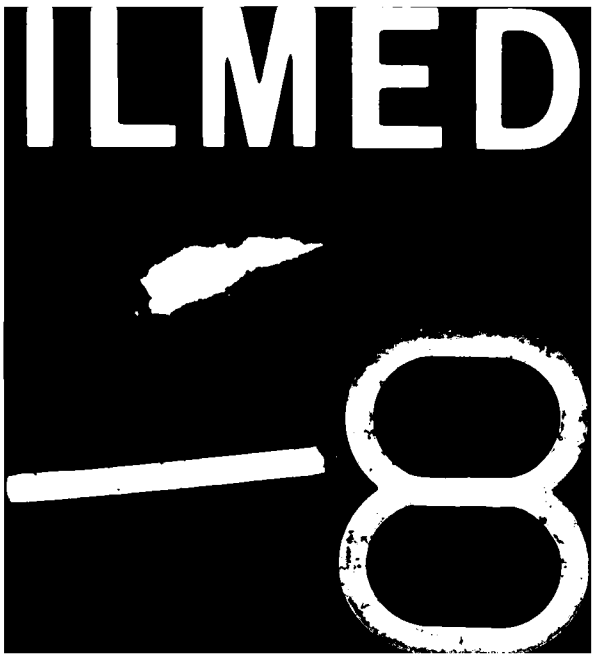
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